Recent advances and applications of deep learning methods in materials science

Year: 2021 | Citations: 793 | Authors: K. Choudhary, Brian L. DeCost, Chi Chen, Anubhav Jain, F. Tavazza

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Abstract

Deep learning (DL) is one of the fastest-growing topics in materials data science, with rapidly emerging applications spanning atomistic, image-based, spectral, and textual data modalities. DL allows analysis of unstructured data and automated identification of features. The recent development of large materials databases has fueled the application of DL methods in atomistic prediction in particular. In contrast, advances in image and spectral data have largely leveraged synthetic data enabled by high-quality forward models as well as by generative unsupervised DL methods. In this article, we present a high-level overview of deep learning methods followed by a detailed discussion of recent developments of deep learning in atomistic simulation, materials imaging, spectral analysis, and natural language processing. For each modality we discuss applications involving both theoretical and experimental data, typical modeling approaches with their strengths and limitations, and relevant publicly available software and datasets. We conclude the review with a discussion of recent cross-cutting work related to uncertainty quantification in this field and a brief perspective on limitations, challenges, and potential growth areas for DL methods in materials science.